

Output from Bose condensates in tunnel arrays: the role of mean-field interactions and of transverse confinement

M. L. Chiofalo ^{*} and M. P. Tosi

*Istituto Nazionale di Fisica della Materia and Classe di Scienze,
Scuola Normale Superiore, I-56126 Pisa, Italy*

Abstract

We present numerical studies of atomic transport in 3D and 1D models for a mode-locked, pulsed atom laser as realized by Anderson and Kasevich [Science 281 (1998) 1686] using an elongated Bose condensate of ^{87}Rb atoms poured into a vertical optical lattice. From our 3D results we ascertain in a quantitative manner the role of mean-field interactions in determining the shape and the size of the pulses in the case of Gaussian transverse confinement. By comparison with 1D simulations we single out a best-performing 1D reduction of the mean-field interactions, which yields quantitatively useful predictions for all main features of the matter output.

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^{*} Corresponding author

Maria Luisa Chiofalo

Scuola Normale Superiore

Piazza dei Cavalieri 7, I-56126 Pisa (Italy)

Tel.: +39-050-509.058

e-mail: marilu@ducky.sns.it

1 Introduction

The dynamics of Bose-Einstein condensates of alkali vapours [1]-[3] in very elongated traps is a matter of wide experimental and theoretical interest. An example is the mode-locked, pulsed atom laser which has been realized by Anderson and Kasevich [4] by pouring a condensate of ^{87}Rb atoms in a vertical optical lattice. Drops of coherent matter leave the condensate under the effect of gravity. In this and other similar situations a theorist would like to reduce the problem to one-dimensional (1D) transport along the axial direction, keeping account of the interactions through a renormalization of the scattering length embodying the transverse confinement of the 3D condensate.

A numerical study of atomic transport in a model relevant to the above-mentioned system has been based on the solution of a 1D time-dependent Gross-Pitaevskii equation (GPE) [5]. This was obtained by freezing out the transverse motions of the condensate and by renormalizing the mean-field interactions according to a proposal made by Jackson *et al.* [6]. The main result of this study was to show that, independently of the strength of the interactions and in complete agreement with the experimental data of Anderson and Kasevich [4], the separation between successive matter drops is determined by the period of Bloch oscillations of the condensate in the 1D periodic potential of the optical lattice. It was further seen from the numerical results that the shape of the drops is closely related to that of the parent condensate, thus supporting a mechanism of coherent emission and suggesting a practical way to tailor matter-wave laser pulses. Nevertheless, the question remains of how far a specific 1D schematization may quantitatively capture other features of the phenomenon.

In this Letter we address this question by carrying out a 3D numerical study of gravity-driven transport in a cylindrically symmetric condensate inside an optical lattice and by testing against these data the results of 1D reductions of the problem. In addition to the proposal of Jackson *et al.* [6], we test a reduction previously proposed for condensates in anisotropic harmonic traps [7, 8], in which we fix the effective 1D scattering length by adjusting the chemical potential of the 1D model to that of the 3D condensate. As a further proof that the phenomenon of drop emission reflects the Bloch oscillations of the condensate, the spacing between the drops remains the same in all these models. The focus of our study then is on the shape and size of the matter

pulses.

In our numerical simulations we use a fast, explicit time-marching scheme for the solution of the GPE in cylindrical geometry, which has been developed by Cerimele *et al.* [9]. This method is briefly described in Section 2. Our extensive results of 3D simulation are presented in Section 3 and summarized in a simple diagram reporting the fractional number of particles in the first drop as a function of a single, suitably defined combination of system parameters. The corresponding results from the 1D reductions are reported in Section 4 and critically compared with those of the 3D simulation in Section 5. This final section also present our conclusions.

2 The numerical method

The time-dependent GPE for the condensate wave function $\Psi(\mathbf{r}, t)$ is [10, 11]

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2M} + U_{ext}(\mathbf{r}) + U_I |\Psi(\mathbf{r}, t)|^2 \right) \Psi(\mathbf{r}, t) \quad , \quad (1)$$

where M is the atomic mass, $U_I = 4\pi\hbar^2 a N / M$ is the interaction strength and U_{ext} is the external potential, a being the scattering length and N the number of particles in the condensate. In what follows $U_{ext}(\mathbf{r})$ is due to the optical lattice and to gravity, namely

$$U_{ext}(r, z) = U_l^0 [1 - \exp(-r^2/r_{lb}^2) \cos^2(2\pi z/\lambda)] - Mgz \quad , \quad (2)$$

Here, U_l^0 is the well depth, r_{lb} is the transverse size, the wavelength λ yields the lattice period $d = \lambda/2$ and g is the acceleration of gravity. Finally, the normalization condition is $\int |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1$.

We numerically solve Eq. (1) by using an *explicit* time marching technique [9], in contrast with alternating-direction-implicit solver methods previously used in the context of Bose-Einstein condensation [12, 13]. The present algorithm extends a fast time-staggered scheme proposed by Visscher [14] to solve the Schrödinger equation in an external potential, with the aims of preserving norm conservation in the presence of non-linear mean-field interactions and of handling cylindrical symmetry [5, 9]. In brief, in solving Eq. (1) we synchronously advance the real and imaginary parts of the scaled wave function in units of two time steps, using their intermediate centred value. The space derivatives are approximated by using centred differentiation.

The following crucial points deserve special comment. It is proven a priori [9] and numerically verified that the algorithm preserves the norm of the wave function at each time step, provided that the boundary conditions are such as to annihilate surface terms. It can also be shown [9] that the numerical stability of the algorithm is preserved as long as the simulation time-step does not exceed a critical value $\Delta\tau_c$, which is limited either by the grid spacing or by the magnitude of the product aN entering U_I . In our simulations the actual time-step is consistently kept well below the marginal stability threshold. Finally, the cylindrical symmetry is handled by an accurate treatment of the space derivatives near the symmetry axis [12].

3 Results for a 3D condensate in cylindrical geometry

Equation (1) is made dimensionless by adopting the scale units $S_l = \sqrt{\hbar/2M\omega}$, $S_t = 1/\omega$ and $S_E = \hbar\omega$ for length, time and energy, ω being the radial frequency of the original magnetic trap. We also rescale the wave function by the dimensionless radial coordinate ρ . We use a grid resolution of 21×16 on each single well, the time step being $\Delta\tau = 2 \cdot 10^{-6}$.

The initial value $\Psi(r, z; t = 0)$ of the wave function is chosen so as to approximate the condensate realized in [4]. Namely,

$$\Psi(r, z; t = 0) = A \exp[-M(\omega_r r^2 + \tilde{\omega} z^2)/2\hbar] \sum_l \exp[-M\omega_z(z - ld)^2/2\hbar] . \quad (3)$$

Here, A is a normalization factor and l labels the occupied sites, their total number being n_w . In constructing Eq. (3) we have assumed (i) constant phase of the condensate in space [15]; (ii) a Gaussian transverse profile with a frequency $\omega_r = \sqrt{2U_l^0/(Mr_{lb}^2)}$ given by the harmonic approximation to the transverse shape of the optical potential; and (iii) an overall axial profile reflecting that of the condensate inside the magnetic trap before loading the optical lattice and taken as a Gaussian having frequency $\tilde{\omega} = 4\pi^{3/5}/\zeta^2\omega$, with $\zeta = (32\pi Na/S_l)^{1/5}$ [16]. Finally, the lowest state at each lattice site is occupied by a portion of condensate, having Gaussian shape with frequency $\omega_z = 2\sqrt{U_l^0 E_R}/\hbar$, where $E_R = \hbar^2/2M\lambda^2$ is the recoil energy.

Before entering the presentation of the simulation results, we list below the system parameters relevant to the experiment on ^{87}Rb [4]. These are

$a = 110a_0$ with a_0 the Bohr radius, $N = 10^4$, $\lambda = 850 \text{ nm}$, $r_{lb} = 80 \text{ }\mu\text{m}$, $U_l^0 = 1.4 E_R$ and $n_w = 31$. The parameters in this reference list provide our reference run.

Fig. 1 shows four pictures of drop emission for different values of the coupling strength, by plotting the contour density profiles, taken with $U_l^0 = 1.4 E_R$ after 5.3 ms . The first panel displays the behaviour of the non-interacting gas, namely the case $a = 0$ and $n_w = 31$. The other panels report the behaviour of the interacting gas with $a = 110 a_0$; from left to right, the cases $N = 10^4$ with $n_w = 31$, $N = 10^5$ with $n_w = 49$ and $N = 2 \cdot 10^5$ with $n_w = 57$. All the other parameters are as listed above.

A number of the results obtained in the earlier 1D simulation [5] are recovered in the present 3D runs. Each drop in figure 1 extends over a number of wells equal to that occupied by the parent condensate. In all cases the drops are equally spaced by seventy wells from centre to centre. This spacing corresponds to 1.1 ms of simulation time, in agreement with experiment [4] and with the value of 1.09 ms for the period $T_B = 2h/Mg\lambda$ of Bloch oscillations of the condensate in the periodic optical potential. The time lag between successive drops is independent of the amplitude of the periodic potential, of the strength of the interactions and of the dimensionality of the simulation sample, as expected if Bloch oscillations provide the correct interpretation of the observations [15]. Finally, both the axial width and the fine structure of each drop reproduce those of the parent condensate, as expected for coherent emission from all lattice wells.

Again in analogy with the case of 1D simulation [5], the transport behaviour of the 3D system as a function of its governing parameters can be summarized in a single diagram. We introduce a scaling parameter g_s , having the dimensions of the acceleration of gravity, by setting

$$Mg_s d = U_l^0 - U_i \quad (4)$$

where $U_i \equiv 4\pi\hbar^2 a N / MR^3$ with $R = \zeta S_l$ is a measure of the mean-field interaction strength. In figure 2 we plot the fractional number N_{drop}/N of atoms in the first drop as a function of the ratio g/g_s , each symbol representing a run with different input parameters. Symbols of different shape represent runs at different values of U_l^0/E_R , as shown in the legend. For each symbol we report the values of N_{drop}/N corresponding to increasing coupling strength U_i , starting from the non-interacting gas and then increasing N in the sequence $N = 10^4$, 10^5 and $2 \cdot 10^5$ (from left to right).

It is seen from figure 2 that there is a critical value for the onset of drop formation, which is $g/g_s \simeq 0.14$ (the onset is marked by an arrow). To all effects there is no emission of drops for subcritical values of g/g_s , since the condition of resonance between the bound state in the well and the continuum is not satisfied. Well defined drops are instead emitted at supercritical values of g/g_s . In this regime N_{drop}/N increases rather regularly with g/g_s and shows little sensitivity to the strength of the mean-field interactions at fixed U_l^0 . Ultimately, with decreasing U_l^0 the potential wells become too shallow and regular drop emission turns into a discharge of the whole condensate.

On the other hand, an increase in the mean-field interactions affects the axial width of the drops. In particular the width of the first drop, as measured by its second moment, is close to $n_w/2$, with an appreciable scatter from case to case, while the centre-to-centre distance of neighbouring drops is about 70 wells. As a result, overlap between drops starts at $N \simeq 3 \cdot 10^5$.

In summary, our 3D simulations confirm that the transport behaviour of a Bose condensate in a vertical optical lattice is described by a diagram as shown in figure 2. This diagram could yield useful predictions even for atomic species different from ^{87}Rb .

4 One-dimensional modelling

The time-dependent GPE for a 1D reduction of the present transport problem is [5]

$$i\hbar \frac{\partial \psi(z, t)}{\partial t} = \left(-\frac{\hbar^2 \nabla_z^2}{2M} + u_{ext}(z) + u_I |\psi(z, t)|^2 \right) \psi(z, t) \quad , \quad (5)$$

where $u_{ext}(z) = U_l^0 \sin^2(2\pi z/\lambda) - Mgz$ and $u_I = 4\pi\hbar^2 \tilde{a}N/M$, \tilde{a} being a renormalized coupling parameter with the dimensions of an inverse length.

In the renormalization proposed by Jackson *et al.* [6] (hereafter referred to as model I) one assumes that the coherence length of the condensate in the axial direction is much larger than its transverse radius. The 3D wave function is factorized as $\Psi(\mathbf{r}, t) = g(r, \sigma(z(t)))$ where $\sigma(z)$ is the axial density. Using a harmonic approximation for the radial part of the optical potential, one obtains in the specific problem an effective scattering length $\tilde{a}^I \equiv \gamma^I a$ with $\gamma^I = \sqrt{U_l^0/E_R}/(r_{lb}\lambda)$. A similar renormalization of U_l^0 is negligible, since $r_{lb} \gg \lambda$.

As an alternative (hereafter referred to as model II) we impose that the value of the chemical potential of the 3D system be preserved upon reduction to 1D [7, 8]. As is shown in a detailed calculation given in Appendix A within the Thomas-Fermi approximation, we find $\tilde{a}^{II} = \gamma^{II}a$ with γ^{II} given (for $U_l^0 > \mu$) by

$$\gamma^{II} = \frac{1}{\pi r_{lb}^2} + \frac{U_l^0 - \mu}{4E_R} \frac{1}{\lambda a N} I(\mu), \quad (6)$$

an explicit expression for the positive quantity $I(\mu)$ being given in the Appendix. We remark for later discussion that γ^{II} in Eq. (6) depends implicitly on the product aN which determines the interaction strength.

Table 1 reports the values of $\gamma^I S_l^2$ and $\gamma^{II} S_l^2$ for a number of values of U_l^0/E_R and of N , all other parameters being as in the reference list. The values of μ/E_R are also shown. The important point of Table 1 is that while γ^I is independent of N , γ^{II} decreases with increasing N . This means that in model I an increase in the number of particles leads to a much more rapid increase of the mean-field interaction parameter. For instance, in the case $U_l^0/E_R = 1.4$ an increase of N by a factor 30 implies that $\gamma^{II}aN$ increases by only a factor 6.8.

In the next Section we discuss the consequences of these different behaviours of the two 1D models. We compare the results of the 3D simulation reported in Section 3 with those obtained by solving the 1D GPE with \tilde{a}^I or \tilde{a}^{II} inserted in turn into the mean-field term u_I .

5 Discussion and concluding remarks

Table 2 collects the results for the fractional number N_{drop}/N of atoms in the first drop for different values of U_l^0/E_R and N in the interacting gas, as calculated from (i) the 3D simulation in cylindrical geometry (third column), (ii) the 1D simulation in model I (fourth column), and (iii) the 1D simulation in model II (last column).

It is immediately seen that model II works better than model I and quantitatively reproduces the data of the 3D simulation. The interactions lift the bound state towards the continuum by an amount which may be measured by the mean interaction energy E_I per particle. This is proportional to the product of the effective scattering length times the particle density. In the 1D simulation according to model I we have $E_I \propto \tilde{a}/\lambda \propto a/\lambda^2 r_{lb}$. In the 3D

simulation we have instead $E_I \propto a/(\lambda r_{lb}^2)$, which is significantly smaller since $r_{lb} \gg \lambda$.

Thus a picture emerges in which axial transport is accompanied by a transverse breathing of the condensate, due to the vanishing of radial confinement at $z = (2n + 1)\lambda/4$ (see Eq. (2)). Model I cannot account for this behaviour, since it has been derived by freezing the transverse motion. It also follows that an increase in coupling strength is partially accommodated by a transverse spreading of the condensate, so that the value of N_{drop}/N is rather insensitive to the mean-field interactions in the present range of system parameters.

In summary, a Bose condensate in an optical lattice, subject to a constant driving field in the linear transport regime, behaves as a coherent blob of matter which executes Bloch oscillations through band states and can undergo Zener tunnel at the Brillouin zone edge. The simple diagram shown in Figure 2 describes the drops of coherent matter which are emitted *via* tunnel into the continuum, in dependence of the governing parameters of the system. The effect of the mean-field interactions is very small within the range of system parameters in which regular pulses are emitted. A quantitative reduction of this behaviour to a 1D model can be achieved by imposing a simple condition of constancy of the chemical potential. We expect that this method of dimensionality reduction will be useful in other similar problems and applications.

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A Calculation of the renormalization factor

γ^{II}

We set $\Psi(\mathbf{r}, t) = \exp(i\mu t/\hbar)\Psi(\mathbf{r})$ in Eq. (1) and $\psi(z, t) = \exp(i\mu t/\hbar)\psi(z)$ in Eq. (5). We then have to solve the stationary GPE's

$$\mu\Psi(\mathbf{r}) = \left(-\frac{\hbar^2\nabla_{\mathbf{r}}^2}{2M} + U_{ext}(\mathbf{r}) + U_I|\Psi(\mathbf{r})|^2\right)\Psi(\mathbf{r}) \quad (\text{A.1})$$

for $\Psi(\mathbf{r})$ in the 3D and

$$\mu\psi(z) = \left(-\frac{\hbar^2\nabla_z^2}{2M} + u_{ext}(z) + u_I|\psi(z)|^2\right)\psi(z) \quad . \quad (\text{A.2})$$

for $\psi(z)$ in 1D. To this end we use the Thomas-Fermi approximation, which amounts to neglecting the kinetic energy terms. We then impose the normalization condition on $\Psi(\mathbf{r})$ and on $\psi(z)$, thereby obtaining the expressions for the chemical potential μ .

After introducing dimensionless quantities as indicated in Section 3 and assuming confinement ($U_l^0 > \mu$), this procedure yields the relations

$$\frac{32\pi^2 a N \gamma^{II} S_l^2}{U_l^0 \lambda} = (1 - 2\beta) \arccos(2\beta - 1) + \sqrt{1 - (2\beta - 1)^2} \quad (\text{A.3})$$

in the 1D case and

$$\frac{32\pi^2 a N S_l^2}{U_l^0 \lambda} = \frac{32\pi^2 a N \gamma^{II} S_l^2}{U_l^0 \lambda} - 2\beta \int_0^{\arccos(2\beta-1)} w \tan(w/2) dw \quad (\text{A.4})$$

in the 3D case, where $\beta \equiv (U_l^0 - \mu)/U_l^0$. These equations yield Eq. (6) in the main text, where

$$I(\mu) = \int_0^{f(\mu)} w \tan(w/2) dw > 0 \quad (\text{A.5})$$

with

$$f(\mu) = \arccos(2(U_l^0 - \mu)/U_l^0 - 1) \quad . \quad (\text{A.6})$$

In our numerical calculations we first determine μ from Eq. (A.1) and then γ^{II} from Eq. (6).

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Figure captions

Fig. 1: Contour plots of the condensate density after 5.3 ms for $U_l^0 = 1.4 E_R$, as functions of the axial coordinate z/d and of the transverse distance in μm . The first panel on the left refers to the non-interacting gas with a number of particles $N = 10^4$. The other panels refer to the interacting gas, for $a = 110 a_0$ and various values of N (from left to right, $N = 10^4$, 10^5 and $2 \cdot 10^5$).

Fig. 2: Diagram for drop formation from 3D simulation in cylindrical geometry. We plot the fractional number N_{drop}/N of particles in the first drop against g/g_s for $g = 981\text{ cm/s}^2$. The meaning of the symbols is explained in the legend and in the text.

U_0/E_R	N	$\gamma^I S_l^2$	$\gamma^{II} S_l^2$	μ/E_R
0.4	10^4	$7.9 \cdot 10^{-2}$	$3.4 \cdot 10^{-3}$	0.11
	10^5		$1.2 \cdot 10^{-3}$	0.25
	$2 \cdot 10^5$		$8.5 \cdot 10^{-4}$	0.31
	$3 \cdot 10^5$		$6.8 \cdot 10^{-4}$	0.34
0.7	10^4	0.10	$4.3 \cdot 10^{-3}$	0.16
	10^5		$1.6 \cdot 10^{-3}$	0.36
	$2 \cdot 10^5$		$1.1 \cdot 10^{-3}$	0.45
	$3 \cdot 10^5$		$9.2 \cdot 10^{-4}$	0.51
1.4	10^4	0.15	$5.7 \cdot 10^{-3}$	0.24
	10^5		$2.1 \cdot 10^{-3}$	0.57
	$2 \cdot 10^5$		$1.6 \cdot 10^{-3}$	0.72
	$3 \cdot 10^5$		$1.3 \cdot 10^{-3}$	0.83
2.1	10^4	0.18	$6.8 \cdot 10^{-3}$	0.31
	10^5		$2.6 \cdot 10^{-3}$	0.73
	$2 \cdot 10^5$		$1.9 \cdot 10^{-3}$	0.94
	$3 \cdot 10^5$		$1.6 \cdot 10^{-3}$	1.08

Table 1: Calculated values of $\gamma^I S_l^2$, $\gamma^{II} S_l^2$ and μ/E_R for various values of U_l^0/E_R and N .

U_0/E_R	N	N_{drop}/N		
		3D	1D Model I	1D Model II
0.7	10^4	0.61	0.60	0.60
	10^5	0.61	0.60	0.61
	$2 \cdot 10^5$	0.61	0.66	0.62
1.4	10^4	0.12	0.12	0.12
	10^5	0.11	0.26	0.11
	$2 \cdot 10^5$	0.11	0.32	0.10
2.1	10^4	0.01	0.01	0.01
	10^5	0.01	0.06	0.01
	$2 \cdot 10^5$	0.007	0.02	0.007

Table 2: Fractional number N_{drop}/N of atoms in the first drop for various values of U_l^0/E_R and N .



